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Development in Drug Discovery

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Drug discovery and development has a long history since the early days of human civilization. In ancient times, drugs were used for physical remedies and also associated with religious and spiritual healing. The early drugs or folk medicines were derived mainly from plant and supplemented by animal products. These drugs were most probably discovered through a combination of trial and error experiments and observation of human and animal reactions as a result of these products.

In ancient time, most of the drugs were based on herbs or extraction of ingredients from botanical sources. The synthetic drugs using chemical methods were indicated at the beginning of the 1900's, and that was the beginning of the pharmaceutical industry. Many drugs were researched and manufactured, but mostly they were used from therapeutic point of view rather than curing the diseases. From the early 1930's, drug discovery focused on screening of natural products and isolating the active ingredients for the treatment of the diseases. The active ingredients are usually the synthetic version of the natural products. These synthetic versions, called the new chemical entities (NCEs), have to go through many tests to ensure their potency and safety.

Despite the many advances made in the 1800's, there were very few drugs available for curing diseases at the beginning of the 1900. In the late 1970's, development of re-

combinant DNA products commenced by utilizing cellular and molecular biology knowledge. The biotechnology field became a reality. The pharmaceutical industry combined with the advances in gene therapy, understanding of the diseases' mechanisms, and the research done from the Human Genome Projects have opened up a variety of opportunities and the possibility of the development and use of drugs specifically targeting the exact site of the disease.

The conclusions made from the human genome project showed an increase number of new therapeutic targets used for drug discovery. Also, the high-throughput protein purification, crystallography and nuclear magnetic resonance spectroscopy techniques have been developed and contributed to many structural details of proteins and protein-ligand complexes. These kind advances allow computational strategies to be used in all aspects of drug discovery in recent years, such as the virtual screening (VS) technique for hit identification and lead optimization methods.

As to structure-based drug design, molecular docking is the most common method to be used these days. Programs based on different algorithms are developed to perform molecular docking studies and have made molecular docking a vital tool in pharmaceutical research at present.